No syntax errors found.
Please wait while processing ....

ANNEXURE-A

CIF dictionary
Interpreting this report

Datablock: BS_RAS244

Bond precision: C-C = 0.0087 A Wavelength=0.71073
Cell: a=16.95(2) b=3.974(6) c=13.92(2)
alpha=90 beta=92.697(18) gamma=90
Temperature : 100 K

	Calculated	Reported
Volume	937(2)	937(2)
Space group	P 21/c	P 21/c
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C8 H7 Br N4	?
Sum formula	C8 H7 Br N4	C8 H7 Br N4
Mr	239.08	239.09
Dx,g cm-3	1.695	1.695
Z	4	4
Mu (mm-1)	4.344	4.344
F000	472.0	472.0
F000'	471.01	
h,k,lmax	20,4,17	20,4,17
Nref	1826	1828
Tmin,Tmax	0.348,0.594	0.347,0.593
Tmin'	0.298	

Correction method= # Reported T Limits: Tmin=0.347 Tmax=0.593 AbsCorr = MULTI-SCAN
Data completeness= 1.001 Theta(max)= 25.989
R(reflections)= 0.0470(1056) wR2(reflections)= 0.1488(1828)
S = 0.801 Npar= 119

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level C

RINTA01_ALERT_3_C The value of Rint is greater than 0.12
Rint given 0.124
PLAT148_ALERT_3_C s.u. on the a - Axis is (Too) Large .... 0.020 Ang.
And 2 other PLAT148 Alerts

PLAT148_ALERT_3_C s.u. on the b - Axis is (Too) Large .... 0.0060 Ang.
PLAT148_ALERT_3_C s.u. on the c - Axis is (Too) Large .... 0.020 Ang.

PLAT341_ALERT_3_C Low Bond Precision on C-C Bonds ..... 0.00871 Ang.

Alert level G

PLAT020_ALERT_3_G The Value of Rint is Greater Than 0.12 ..... 0.124 Report
PLAT066_ALERT_1_G Predicted and Reported Tmin&Tmax Range Identical ? Check
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary . Please Do !
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min). 1 Note
PLAT955_ALERT_1_G Reported (CIF) and Actual (FCF) Lmax Differ by . 1 Units
PLAT965_ALERT_2_G The SHELXL WEIGHT Optimisation has not Converged Please Check
PLAT967_ALERT_5_G Note: Two-Theta Cutoff Value in Embedded .res .. 52.0 Degree
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 0 Info

0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
5 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
8 **ALERT level G** = General information/check it is not something unexpected

3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
2 ALERT type 2 Indicator that the structure model may be wrong or deficient

```
   7 ALERT type 3 Indicator that the structure quality may be low
   0 ALERT type 4 Improvement, methodology, query or suggestion
   1 ALERT type 5 Informative message, check
```

It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the purpose of your study may justify the reported deviations and the more serious of these should normally be commented upon in the discussion or experimental section of a paper or in the "special_details" fields of the CIF. checkCIF was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

Publication of your CIF in IUCr journals

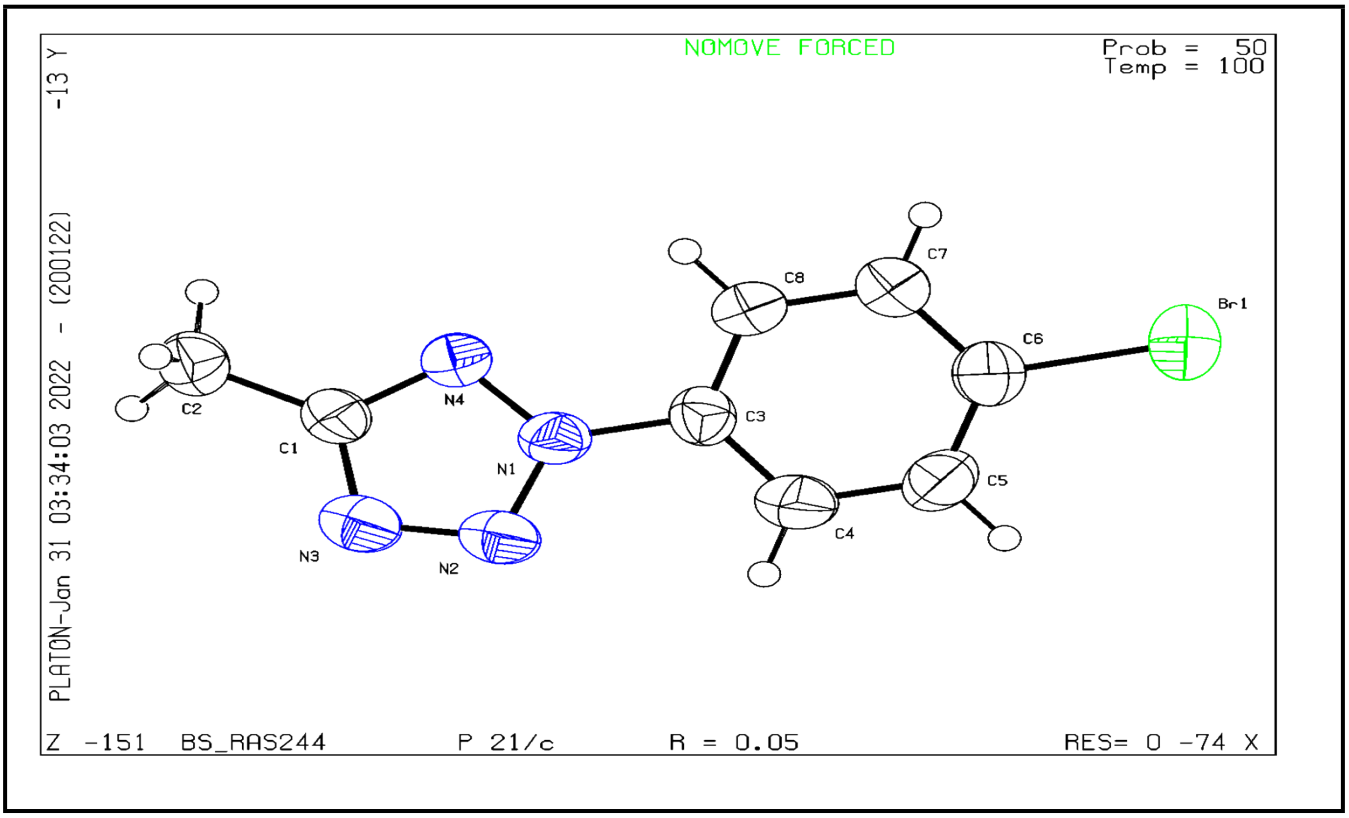
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E* or *IUCrData*, you should make sure that full publication checks are run on the final version of your CIF prior to submission.

Publication of your CIF in other journals

Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

PLATON version of 20/01/2022; check.def file version of 19/01/2022

Datablock BS_RAS244 - ellipsoid plot



Download CIF editor (publCIF) from the IUCr
Download CIF editor (enCIFer) from the CCDC
Test a new CIF entry

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) bs_kt87

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: bs_kt87

```
Bond precision:   C-C = 0.0039 A          Wavelength=0.71073

Cell:             a=11.542(13)      b=14.958(16)        c=7.936(9)
                  alpha=90          beta=106.50(2)      gamma=90
Temperature:      100 K

                 Calculated                Reported
Volume           1314(3)                   1314(3)
Space group      P 21/c                    P 21/c
Hall group       -P 2ybc                   -P 2ybc
Moiety formula   C16 H13 N O3              ?
Sum formula      C16 H13 N O3              C16 H13 N O3
Mr               267.27                    267.27
Dx,g cm-3        1.351                     1.351
Z                4                         4
Mu (mm-1)        0.094                     0.094
F000             560.0                     560.0
F000'            560.28
h,k,lmax         14,18,9                   14,18,9
Nref             2580                      2580
Tmin,Tmax        0.977,0.988               0.976,0.987
Tmin'            0.976

Correction method= # Reported T Limits: Tmin=0.976 Tmax=0.987
AbsCorr = MULTI-SCAN

Data completeness= 1.000          Theta(max)= 26.000

R(reflections)= 0.0612( 1842)                wR2(reflections)=
                                             0.1637( 2580)
S = 1.057                 Npar= 183
```

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level B

PLAT196_ALERT_1_B No TEMP record and _measurement_temperature .NE. 293 Degree
PLAT919_ALERT_3_B Reflection # Likely Affected by the Beamstop ... 1 Check

Alert level C

PLAT148_ALERT_3_C s.u. on the a - Axis is (Too) Large .... 0.013 Ang.
PLAT148_ALERT_3_C s.u. on the b - Axis is (Too) Large .... 0.0160 Ang.
PLAT148_ALERT_3_C s.u. on the c - Axis is (Too) Large .... 0.009 Ang.
PLAT934_ALERT_3_C Number of (Iobs-Icalc)/Sigma(W) > 10 Outliers .. 1 Check

Alert level G

PLAT066_ALERT_1_G Predicted and Reported Tmin&Tmax Range Identical ? Check
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary . Please Do !
PLAT965_ALERT_2_G The SHELXL WEIGHT Optimisation has not Converged Please Check
PLAT967_ALERT_5_G Note: Two-Theta Cutoff Value in Embedded .res .. 52.0 Degree
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 0 Info

0 **ALERT level A** = Most likely a serious problem - resolve or explain
2 **ALERT level B** = A potentially serious problem, consider carefully
4 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
5 **ALERT level G** = General information/check it is not something unexpected

3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
2 ALERT type 2 Indicator that the structure model may be wrong or deficient
5 ALERT type 3 Indicator that the structure quality may be low
0 ALERT type 4 Improvement, methodology, query or suggestion
1 ALERT type 5 Informative message, check

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Publication of your CIF in IUCr journals

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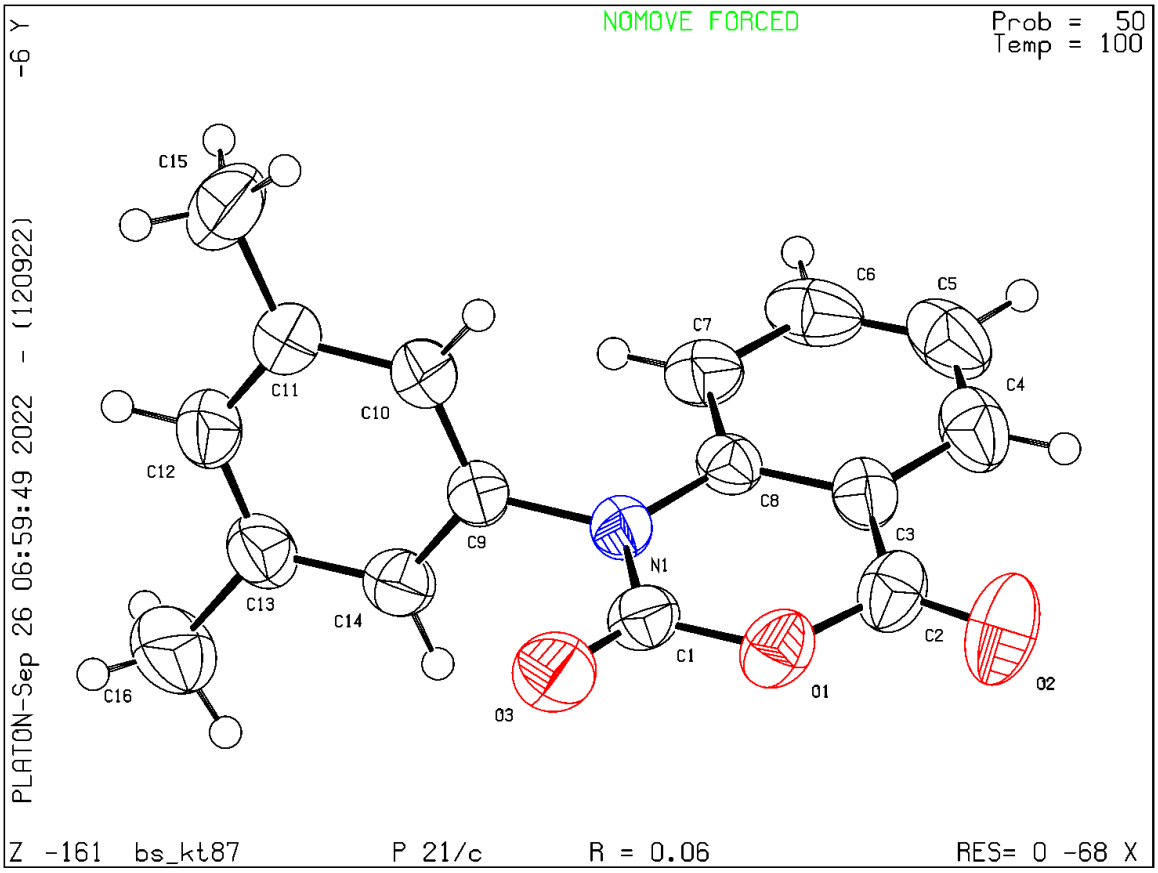
Publication of your CIF in other journals

Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

PLATON version of 12/09/2022; check.def file version of 09/08/2022

Datablock bs_kt87 - ellipsoid plot



checkCIF/PLATON report

Structure factors have been supplied for datablock(s) BS_4OME

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: BS_4OME

```
Bond precision:   C-C = 0.0060 A          Wavelength=0.71073

Cell:                a=14.12(5)       b=11.00(4)       c=16.65(6)
                     alpha=90         beta=90          gamma=90
Temperature:         100 K
```

	Calculated	Reported
Volume	2586(16)	2587(15)
Space group	P b c a	P b c a
Hall group	-P 2ac 2ab	-P 2ac 2ab
Moiety formula	C15 H11 N O4	?
Sum formula	C15 H11 N O4	C15 H11 N O4
Mr	269.25	269.25
Dx,g cm-3	1.383	1.383
Z	8	8
Mu (mm-1)	0.102	0.102
F000	1120.0	1120.0
F000'	1120.62	
h,k,lmax	17,13,20	17,13,20
Nref	2542	2544
Tmin,Tmax	0.972,0.988	0.971,0.986
Tmin'	0.968	

```
Correction method= # Reported T Limits: Tmin=0.971 Tmax=0.986
AbsCorr = MULTI-SCAN

Data completeness= 1.001           Theta(max)= 25.997

R(reflections)= 0.0430( 1802)                    wR2(reflections)=
                                                 0.1073( 2544)
S = 0.997                 Npar= 182
```

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level C

PLAT148_ALERT_3_C s.u. on the a - Axis is (Too) Large .... 0.050 Ang.
PLAT148_ALERT_3_C s.u. on the b - Axis is (Too) Large .... 0.0400 Ang.
PLAT148_ALERT_3_C s.u. on the c - Axis is (Too) Large .... 0.060 Ang.
PLAT340_ALERT_3_C Low Bond Precision on C-C Bonds ..... 0.006 Ang.

Alert level G

PLAT066_ALERT_1_G Predicted and Reported Tmin&Tmax Range Identical ? Check
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary . Please Do !
PLAT965_ALERT_2_G The SHELXL WEIGHT Optimisation has not Converged Please Check
PLAT967_ALERT_5_G Note: Two-Theta Cutoff Value in Embedded .res .. 52.0 Degree
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 0 Info

0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
4 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
5 **ALERT level G** = General information/check it is not something unexpected

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0 ALERT type 4 Improvement, methodology, query or suggestion
1 ALERT type 5 Informative message, check

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Publication of your CIF in other journals

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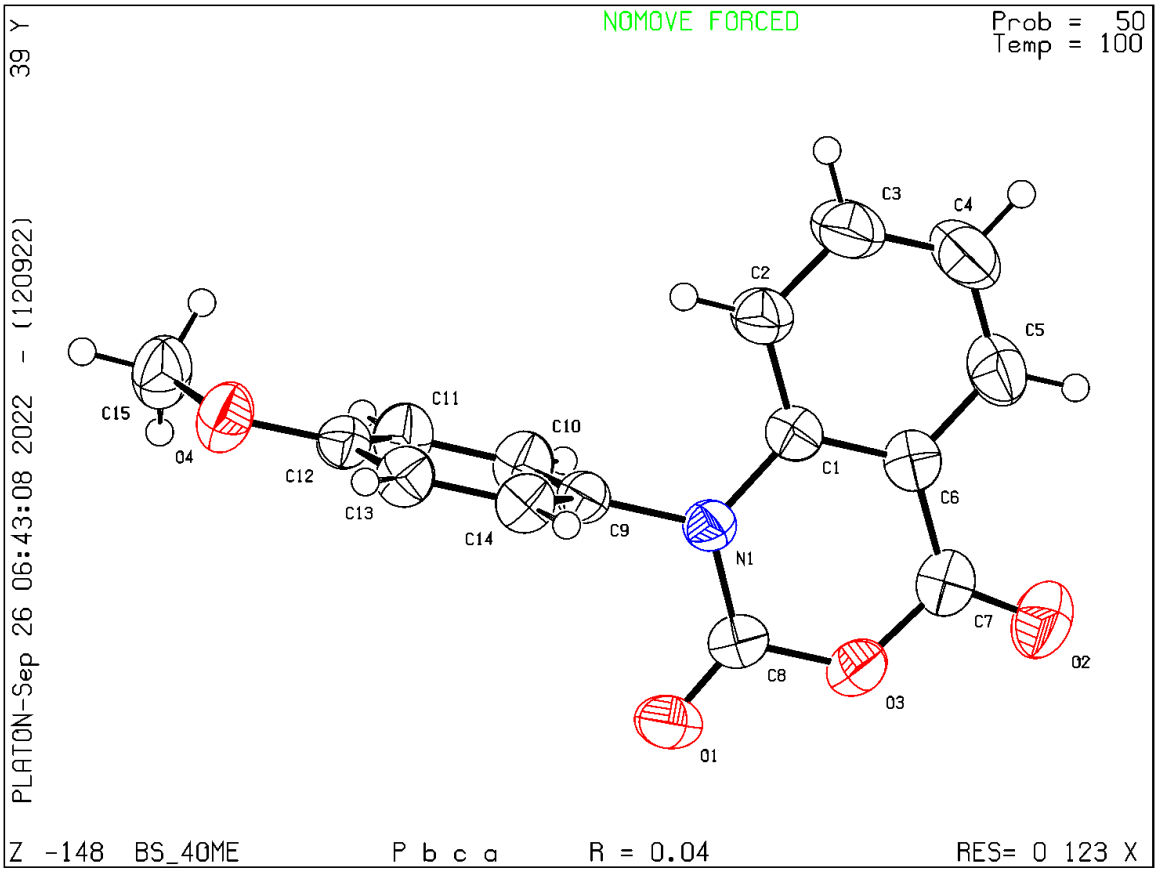
PLATON version of 12/09/2022; check.def file version of 09/08/2022

Datablock BS_4OME - ellipsoid plot



k

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) BS_RAS105_0m_a

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: BS_RAS105_0m_a

```
Bond precision:   C-C = 0.0031 A          Wavelength=0.71073

Cell:             a=9.4144(17)     b=12.311(2)          c=13.869(3)
                  alpha=90         beta=100.021(5)      gamma=90
Temperature:      296 K

                 Calculated                Reported
Volume           1582.9(5)                 1582.9(5)
Space group      P 21/c                    P 21/c
Hall group       -P 2ybc                   -P 2ybc
Moiety formula   C19 H13 F N2 O            ?
Sum formula      C19 H13 F N2 O            C19 H13 F N2 O
Mr               304.31                    304.31
Dx,g cm-3        1.277                     1.277
Z                4                         4
Mu (mm-1)        0.088                     0.088
F000             632.0                     632.0
F000'            632.30
h,k,lmax         11,15,17                  11,15,17
Nref             3109                      3110
Tmin,Tmax        0.973,0.984               0.971,0.980
Tmin'            0.972

Correction method= # Reported T Limits: Tmin=0.971 Tmax=0.980
AbsCorr = MULTI-SCAN

Data completeness= 1.000           Theta(max)= 25.999

R(reflections)= 0.0434( 1941)                wR2(reflections)=
                                             0.1216( 3110)
S = 1.013                Npar= 209
```

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level C

```
PLAT230_ALERT_2_C Hirshfeld Test Diff for    C15      --C16      .        5.5 s.u.
PLAT334_ALERT_2_C Small <C-C> Benzene Dist.   C8       -C13      .       1.37 Ang.
```

Alert level G

```
PLAT066_ALERT_1_G Predicted and Reported Tmin&Tmax Range Identical          ? Check
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .     Please Do !
PLAT967_ALERT_5_G Note: Two-Theta Cutoff Value in Embedded .res ..       52.0 Degree
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.          2 Info
```

0 **ALERT level A** = Most likely a serious problem - resolve or explain
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4 **ALERT level G** = General information/check it is not something unexpected

2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
3 ALERT type 2 Indicator that the structure model may be wrong or deficient
0 ALERT type 3 Indicator that the structure quality may be low
0 ALERT type 4 Improvement, methodology, query or suggestion
1 ALERT type 5 Informative message, check

Validation response form

Please find below a validation response form (VRF) that can be filled in and pasted into your CIF.

```
# start Validation Reply Form
_vrf_PLAT230_BS_RAS105_0m_a
;
PROBLEM: Hirshfeld Test Diff for    C15      --C16      .        5.5 s.u.
RESPONSE: ...
;
_vrf_PLAT334_BS_RAS105_0m_a
;
PROBLEM: Small <C-C> Benzene Dist.   C8       -C13      .       1.37 Ang.
RESPONSE: ...
;
# end Validation Reply Form
```

It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the purpose of your study may justify the reported deviations and the more serious of these should normally be commented upon in the discussion or experimental section of a paper or in the "special_details" fields of the CIF. checkCIF was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

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Publication of your CIF in other journals

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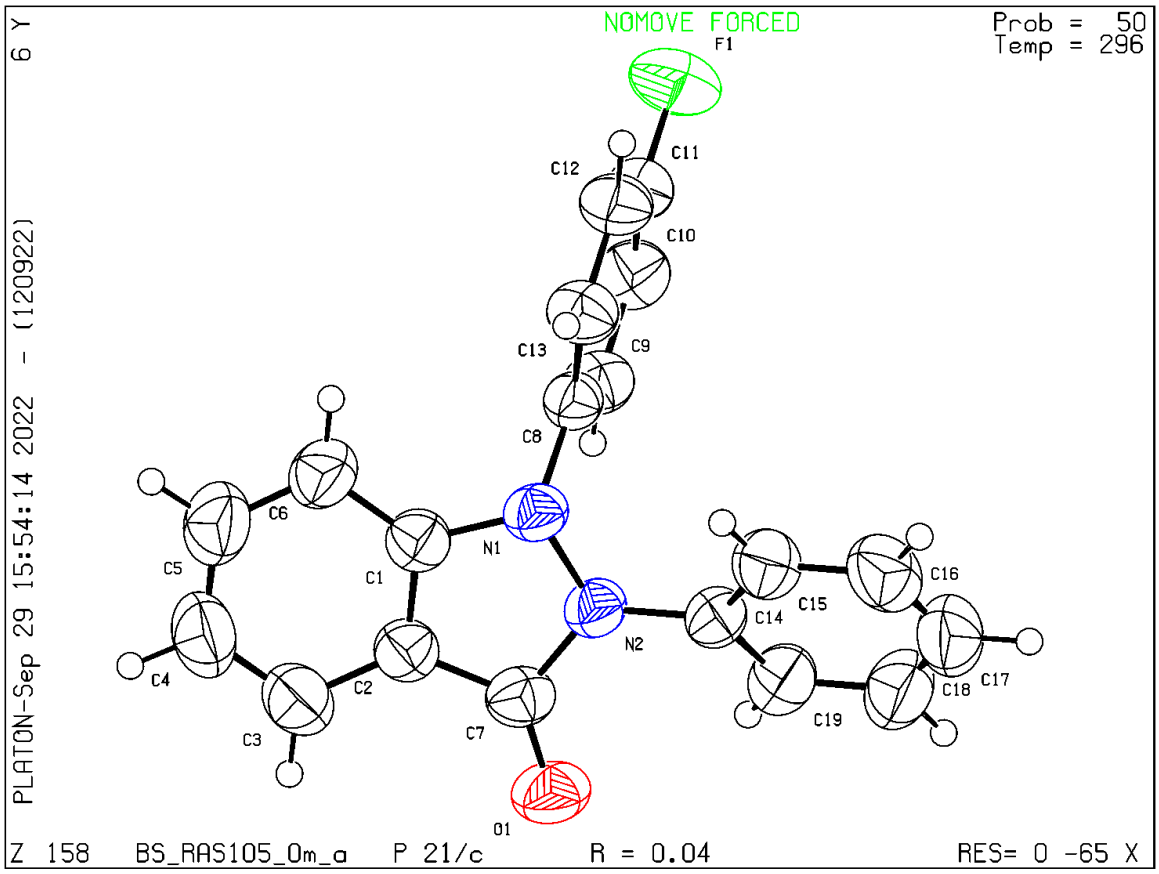
PLATON version of 12/09/2022; check.def file version of 09/08/2022

Datablock BS_RAS105_0m_a - ellipsoid plot



ANNEXURE-E

List of Publications

Journals:

[1] **Saikia, R. A.**, Barman, D., Dutta, A. and Thakur, A. J. N^1-and N^3-Arylations of Hydantoins Employing Diaryliodonium Salts via Copper-(I) Catalysis at Room Temperature. *European Journal of Organic Chemistry*, 2021(3):400-410, 2021. *(https://mjl.clarivate.com:/search-results?issn=1434-193X&hide_exact_match_fl=true&utm_source=mjl&utm_medium=share-by-link&utm_campaign=search-results-share-this-journal)*

[2] **Saikia, R. A.**, Hazarika, N., Biswakarma, N., Deka, R. C. and Thakur, A. J. Metal-free *S*-arylation of 5-mercaptotetrazoles and 2-mercaptopyridine with unsymmetrical diaryliodonium salts. *Organic & Biomolecular Chemistry*, 20(19):3890-3896, 2022. *(https://mjl.clarivate.com:/search-results?issn=1477-0520&hide_exact_match_fl=true&utm_source=mjl&utm_medium=share-by-link&utm_campaign=search-results-share-this-journal)*

[3] **Saikia, R. A.**, Dutta, A., Sarma, B. and Thakur, A. J. Metal-Free Regioselective N^2-Arylation of 1*H*-Tetrazoles with Diaryliodonium Salts. *The Journal of Organic Chemistry*, 87(15):9782-9796, 2022. (*https://mjl.clarivate.com:/search-results?issn=0022-3263&hide_exact_match_fl=true&utm_source=mjl&utm_medium=share-by-link&utm_campaign=search-results-share-this-journal*)

[4] **Saikia, R. A.**, Talukar, K., Pathak, D., Sarma, B. and Thakur, A. J. Utilization of Aryl(TMP)iodonium Salts for Copper-catalyzed *N*-Arylation of Isatoic Anhydrides: An Avenue to fenamic acid derivatives and *N,N′*-diarylindazol-3-ones. *The Journal of Organic Chemistry* (just accepted, DOI: 10.1021/acs.joc.2c02762). (*https://mjl.clarivate.com:/search-results?issn=0022-3263&hide_exact_match_fl=true&utm_source=mjl&utm_medium=share-by-link&utm_campaign=search-results-share-this-journal*)

[5] Dutta, A., **Saikia, R. A.** and Jyoti Thakur, A. A Mechanistic Approach to Liquid-Assisted Mechanochemical Synthesis of 5-Aryl/Spiro-[1,2,4]-triazolidine-3-thiones. *European Journal of Organic Chemistry*, 2022(34):e202101472, 2022. *(https://mjl.clarivate.com:/search-results?issn=1434-193X&hide_exact_match_fl=true&utm_source=mjl&utm_medium=share-by-link&utm_campaign=search-results-share-this-journal)*

[6] Borah, M. J., Devi, A., **Saikia, R. A.** and Deka, D. Biodiesel production from waste cooking oil catalyzed by *in-situ* decorated TiO_2 on reduced graphene oxide

nanocomposite. *Energy*, 158:881-889, 2018. *(https://mjl.clarivate.com:/search-results?issn=0360-5442&hide_exact_match_fl=true&utm_source=mjl&utm_medium=share-by-link&utm_campaign=search-results-share-this-journal)*

Book Chapter:

[1] **Saikia, R. A.** and Saikia, R. A study on organic solvents: Its necessity, its impact on the environment and sustainable alternatives. In Narzary, A., Begum, P. and Bhagawati, C., editors, *Environment: Climate Change and Natural Challenges*, pages 22-41, ISBN: 978-93-90919-60-4. Gargaon College Publication Cell & Purbayon Publication, 2021.

[2] **Saikia, R. A.** 2-iodoxybenzoic Acid (IBX): An Organohypervalent Iodine Compound as Mainstream Oxidant in Organic Synthesis. In Mahanta, S. M. and Kalita, D., editors, *Aspects of Sustainable Chemical Sciences*, pages 98-117, ISBN: 978-93-89940-82-4. Purbayon Publication, 2020.

ANNEXURE-E

List of Conferences

As Abstract

Oral Presentation:

[1] **Saikia R. A.** and Thakur, A. J. *N-arylations of Hydantoins Employing Diaryliodonium Salts via Copper(I) Catalysis at Room Temperature*. International Conference (Virtual) on The Present and Future of Excellence in Organic Synthesis (PFEOS-2021), Organized by Department of Chemical Sciences, Tezpur University, Tezpur, 7th-8th January 2021.

[2] **Saikia R. A.**, and Thakur, A. J. *Room Temperature Copper-Catalyzed N-Arylations of Hydantoins employing Diaryliodonium Salts*. National Seminar on Science for Sustainable Development (SSD-2020), Organized by Department of Chemistry, B. Borooah College, Guwahati, 25th-26th September 2020.

Poster Presentation:

[1] **Saikia, R. A.**, Barman, D., Dutta, A. and Thakur, A. J. *Copper-Catalyzed N-Arylations of Hydantoins with Diaryliodonium Salts*. International Conference on Emerging Trends in Chemical Sciences (ETCS 2020), Organized by Department of Chemistry, Gauhati University, Guwahati, 13th-15th February 2020.

[2] **Saikia, R. A.**, and Thakur, A. J. *Copper-Catalyzed N-Arylations of Hydantoins employing Diaryliodonium Salts at Room Temperature.* First virtual J-NOST symposium; XVI-J-NOST, Organized by Indian Institute of Science, Bangalore, 31st October-1st November 2020.